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The analysis of spin hamiltonian and crystal field tensors for Fe³⁺ in crystals of LiCaAlF₆ and LiSrAlF₆

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Abstract

In single crystals of LiCaAlF₆ and LiSrAlF₆ doped with Fe³⁺ the trigonal EPR spectra with multiplicity $KM = 1$ were observed due to Fe³⁺ substituted for Al³⁺. The spin Hamiltonian parameters describing the fine structure and the superhyperfine structure were determined. It is argued that the tensors B₂ and B₄ of the spin Hamiltonian for Fe³⁺ ions are essentially determined by the quadratic contributions of the crystal field at the substitution site. The signs and the relative values of the elements in the spin Hamiltonian tensor B₄ of rank $L = 4$ for Fe³⁺ are determined by the irreducible tensor product $[V_4 \otimes V_4]_2$ of the crystal field tensor V₄ of rank $L = 4$ at the substitution sites. The ratio between the invariant sum of the spin Hamiltonian tensor B₄ for Fe³⁺ in oxygen octahedra [FeO₆] and that in fluorine octahedra [FeF₆] is directly proportional to the fourth power of the ratio between the effective charges of surrounding ions. The sign of the spin Hamiltonian parameter B₂₀ corresponds to the sign of the element $[V_4 \otimes V_4]_{20}$ in the irreducible tensor product $[V_4 \otimes V_4]_2$ of rank $L = 2$. © Springer-Verlag 1998.
